

# Jacob O. Spiegel, Ph.D.

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## Education

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### University of Pittsburgh

2014 – 2020

#### Ph.D in Molecular Biophysics and Structural Biology

Pittsburgh, PA

- Thesis title: “Targeting the Poly (ADP-Ribose) Polymerase-1 Catalytic Pocket Using AutoGrow4, a Genetic Algorithm for *De Novo* Design”

#### Ph.D Minor in Teaching

### Carnegie Mellon University

2013 – 2014

#### Ph.D. Student in Molecular Biophysics and Structural Biology

Pittsburgh, PA

### Stony Brook University

2009 – 2013

#### B.Eng. in Biomedical Engineering - Cellular and Molecular Biology Track

Stony Brook, NY

## Research Experience

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### University of Pittsburgh

2013 – 2020

#### Ph.D. Candidate/Researcher in Dr. Jacob Durrant's laboratory

Pittsburgh, PA

- Designed, developed, documented, and maintained multiple Python open-source programs for computer-aided drug designed (CADD) and cheminformatics; parallelized code for multiprocessing
- Applied CADD techniques to biological targets; performed molecular dynamic (MD) and weighted ensemble MD simulations on multiple proteins; performed protein homology modeling
- Completed independent and collaborative projects
- Authored scientific articles for publication
- Mentored, managed, and designed projects for/with undergraduate and graduate students

#### Ph.D. Candidate in Dr. Roger Hendrix's laboratory

- Studied bacteriophages using biochemical, molecular genetic, and X-ray crystallography techniques
- Engineered plasmids; designed protein purification protocols; purified proteins for X-ray crystallography

### Stony Brook University

2011 – 2013

#### Undergraduate Researcher in Dr. Balaji Sitharaman's laboratory

Stony Brook, NY

- Studied nanoparticle drug delivery system targeting cancer cells
- Designed alternative exfoliation protocol to produced graphene sheets from graphite

### Cold Spring Harbor Laboratory

2007 – 2010

#### Researcher in Dr. Jonathan Sebat's laboratory

Woodbury, NY

- Semi-Finalist, Intel Science Talent Search
- Designed and conducted independent population genetic study
- Performed microarray experiments searching for polymorphism in autism, bipolar disorder, and schizophrenia patients

## Publications

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### Peer-Reviewed Articles

- **Spiegel, J.O.**, Durrant, J.D. AutoGrow4: an open-source genetic algorithm for *de novo* drug design and lead optimization. J Cheminform 12, 25 (2020). <http://doi.org/ggwwcp>
- Ropp, P.J., **Spiegel, J.O.**, et al. Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. J Cheminform 11, 34 (2019). <http://doi.org/gf48dh>

### Articles in Preparation

- **Spiegel, J.O.**, O'Donnell, A., Durrant, J.D., (2020). Molecular dynamics of  $\alpha$ -arrestin TXNIP.
- **Spiegel, J.O.**, Durrant, J.D., (2020). Mechanism and Pharmaceutical Intervention of Poly (ADP-ribose) polymerase 1 (PARP-1).
- **Spiegel, J.O.**, Durrant, J.D., Bowman, R., O'Donnell, A. (2020). Putting the brakes on  $\alpha$ -arrestin trafficking:  $\alpha$ -arrestin regulation by phosphorylation and ubiquitination.

## Awards

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### Abe and Jean Comensky Memorial Scholarship

2019

**Amdursky Scholarship** 2019

**Biomedical Graduate Student Association Travel Award University of Pittsburgh** 2018

- Awarded for oral presentation at RDKit UGM 2018 at Cambridge University, Cambridge, England

## Conference Presentations

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### Oral Presentations

- **Spiegel, J.O.**, Ropp, P.J., and Durrant, J.D. "Autogrow 4.0: Improved Genetic Algorithm for *de novo* Computer Aided Drug Design" Oral presentation at the RDKit UGM 2018, Cambridge University, Cambridge England September 20, 2018
- **Spiegel, J.O.**, Ropp, P.J., and Durrant, J.D. "Autogrow 4.0: Improved Genetic Algorithm for *de novo* Computer Aided Drug Design" Oral presentation at the MBSB 2018 Symposium, University of Pittsburgh, Pittsburgh PA May 18, 2018

### Poster Presentations

- **Spiegel, J.O.**, Ropp, P.J., and Durrant, J.D. "Autogrow 4.0: Improved Genetic Algorithm for *de novo* Computer Aided Drug Design" Poster presentation at the MBSB 2019 Symposium, University of Pittsburgh, Pittsburgh PA May 13, 2019
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. "Structure determination of  $\lambda$  Tail Assembly Chaperone" Poster presentation at the XXV 2017 Conference on Phage and Virus Assembly, Ellicott City, Maryland August 23, 2017
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. "Structure determination of  $\lambda$  Tail Assembly Chaperone" Poster presentation at the MBSB 2017 Symposium, University of Pittsburgh, Pittsburgh PA May 19, 2017
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. "Structure of  $\lambda$  Tail Assembly Chaperone" Poster presentation at the MBSB 2016 Symposium, University of Pittsburgh, Pittsburgh PA May 13, 2016
- **Spiegel, J.O.**, Duda, R., and Hendrix, R. " $\Phi$ Hau3 Ribosomal Bypass Mechanism" Poster presentation at the MBSB 2015 Symposium, University of Pittsburgh, Pittsburgh PA May 15, 2015

## Leadership and Outreach

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**Sigma Phi Delta Engineering Fraternity** 2010 – 2020

- International Scholastic Development Manager
- Founding member of the Beta-Eta Chapter at Stony Brook University
- Rush Chairman, Sergeant at Arms, Alumni Relations Manager, Risk Reduction Manager, Initiate Education and Academic Chairman

**Mars Elementary School Science Fair** 2018 – 2019

- Volunteer judge at Mars Elementary School Science Fair 2018 & 2019 Mars, PA

**Engineers Without Borders USA** 2010 – 2013

- Founding Member of the Stony Brook University chapter
- Project Development Manager

## Teaching Experience

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### University of Pittsburgh

2018 – 2020  
Pittsburgh, PA

#### Ph.D. Minor in Teaching (2018-2020)

- A two-year graduate-level program. The program included pedagogy training, teaching mentoring, and teaching experience

#### Guest Lecturer: Computational Biology Research (January 31, 2020)

- A three-hour long lecture of 25 students. Designed lesson plan and homework assignment, administered lesson and coordinated in-class discussion using active learning techniques, and designed exam questions for the final
- Course covered an intermediate level of Python coding, with focuses in using third-party APIs including RDKit, Numpy, and Scipy. This lesson also detailed Python Enhancement Proposals (PEP) practices and introduced the core concepts of cheminformatics

#### Undergraduate Research Mentor (Fall 2018 – Fall 2019)

- Held weekly supervision meetings, assisted in project design and code reviews culminating in mentee's authorship on the Gypsum-DL paper (2019)

#### Guest Lecturer: Computational Biology (March 21, 2019)

- Hour long lecture of 25 students. Designed lesson plans and homework assignments, administered lessons and coordinated in-class discussion using active learning techniques, and designed exam questions for the final
- Course covered protein druggability, tools for predicting project success rate, rare and tropical diseases, drug toxicity, drug specificity

#### Graduate Teaching Assistant: Biochemistry Lab (Spring 2019)

- Two separate lab sessions of a combined 38 students. Designed lectures and experiments for the class, designed assignments, graded notebooks and assignments, and prepared materials for in-class experiments
- Course covered aseptic technique, cloning, fusion protein construct, protein induction in E. coli, protein purification, gel electrophoresis, lab notebooks

#### Graduate Teaching Assistant: Macromolecular Structure and Function (Fall 2018)

- Weekly lectures and four separate recitation sections for 100 students. Designed lectures and lesson plans, managed undergraduate teaching assistants, and graded papers
- Course covered fundamentals of structural biology, enzyme catalysis, proteomics, fundamentals of biochemistry

#### Guest Lecture: Biochemistry Lab (February 26, 2018)

- Two hour-long lectures with a total of 38 students. Designed lesson plans and homework assignments, administered lessons
- Lesson was to overview virology, focusing on the classification of virus, viral structure and function, and describe the phage HK97, which students would be studying throughout the semester.

#### Graduate Teaching Assistant: Biochemistry Lab (Spring 2018)

- Two lab sessions with a total of 38 students. Designed lectures and experiments for the class, designed assignments, graded notebooks and assignments, and prepared materials for in-class experiments
- Course covered phage biology, aseptic technique, cloning, fusion protein construct, protein induction in E. coli, protein purification, gel electrophoresis, lab notebooks

### Carnegie Mellon University

2014 – 2014  
Pittsburgh, PA

#### Graduate Teaching Assistant: Virology (Spring 2014)

- Class of 50 students. Conducted recitations, aided in lectures, and graded assignments and exams.
- Course covered bacteriophage biology, mammalian virology, lytic/lysogenic states, virus-caused diseases